Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Seminar

Altermagnetism: A case study of two probable candidates Bulk Orthorhombic $BiFeO_3$ and $CaMnO_3$

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Magnetism stands as a cornerstone in condensed matter physics, playing a crucial role in various technological advancements. Magnetic solids are typically divided into two broad categories: ferromagnet (FM) and antiferro-magnet (AFM). FM exhibits a net magnetisation order parameter in direct space, leading to intriguing phenomena stemming from the electronic spin split band structure in the reciprocal space that breaks the time reversal ($\mathcal{T}$) symmetry in the non-relativistic (NR) limit. On the contrary, in a conventional AFM, due to the compensating antiparallel magnetic ordering, resulting in negligible small macroscopic magnetisation, implying the absence of spin split band structure, thereby preserving the $\mathcal{T}$ symmetry in reciprocal space in the NR limit. However, recent research has sparked a growing interest in exploring the $\mathcal{T}$ reversal symmetry-breaking macroscopic phenomena and the existence of NR spin-splitting, characteristics typically associated with FM, in compounds with vanishingly small magnetisation, which is characteristic of AFM. This abundant and previously unexplored magnetic phase has been termed Altermagnet (AM). Intriguingly, we identify two centrosymmetric materials, bulk orthorhombic $BiFeO_3$ (BFO) and $CaMnO_3$ (CMO), that exhibit such NR spin-splitting phenomena. Through Density Functional Theory (DFT), we unveil an insulating state in both compounds with a preferred AFM order. Our DFT calculations and the magnetic space group (MSG) symmetry analysis in the NR limit uncover a substantial spin splitting phenomena observed only in the k_y-k_z plane in the Brillouin zone (BZ) for both compounds. In contrast, the spin degeneracy is maintained in the k_x-k_y and k_x-k_z planes, respectively. Using the invariant theory, we also formulate the governing Hamiltonian for the spin split pair of bands near the high symmetry Γ point. In this presentation, I will briefly provide an overview of altermagnetism and its distinctions from the other two conventional magnetic phases. Further, I will discuss our DFT findings and symmetry analysis that supports our DFT results in detail. Our finding unequivocally designates these two compounds as promising candidates for altermagnetism, making them promising for technological application.

Thursday, Mar 21st 2024

16:00 Hrs (Tea / Coffee 15:45 Hrs)

Seminar Hall, TIFR-H